Supplementary information

MetaParticles: Computationally engineered nanomaterials with tunable and responsive properties

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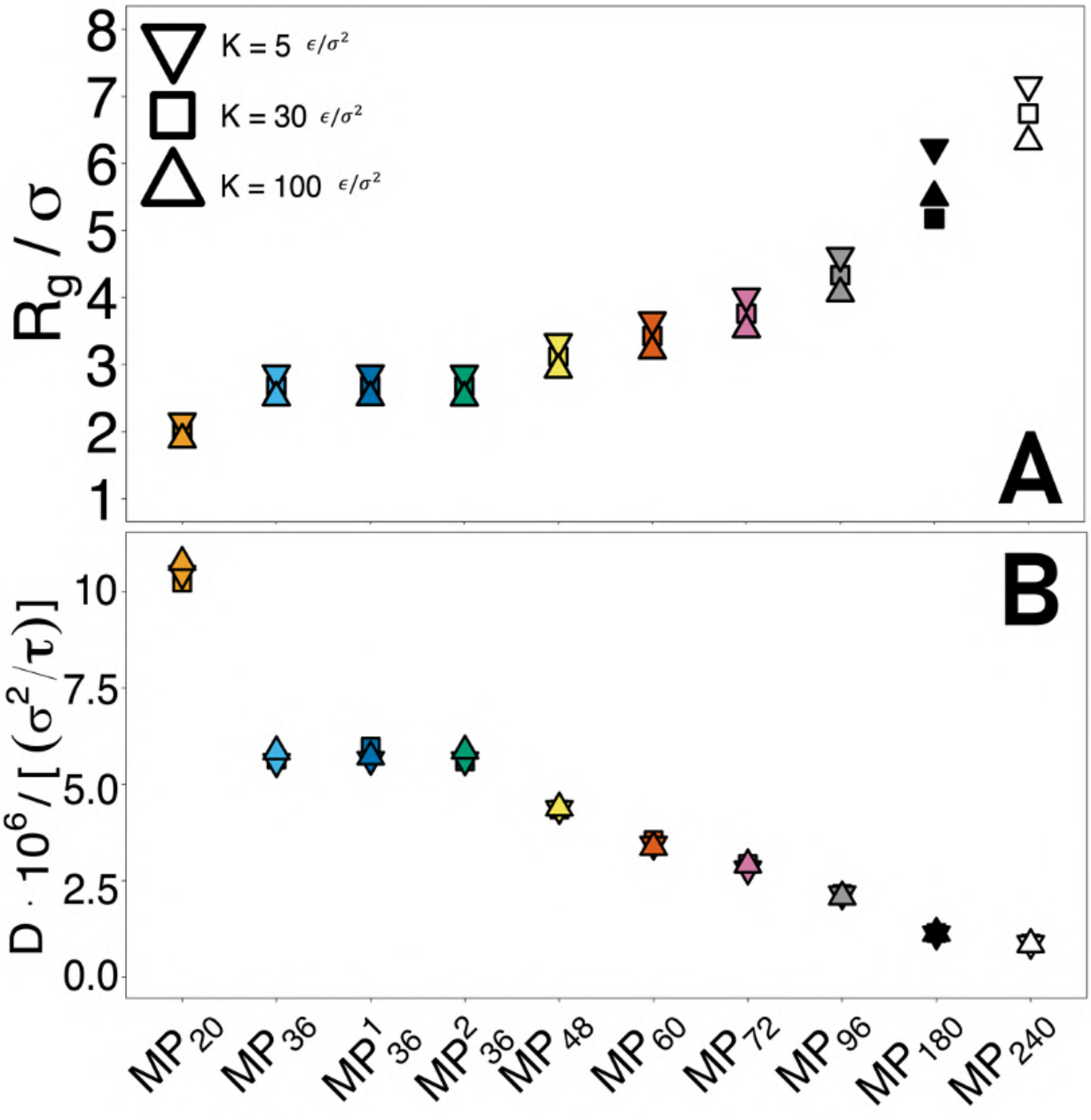

Fig. S1. **(A) Average radii of gyration.** Compared here are the values of the radii of gyration for K = 5 ε/σ^2 (triangles pointing down), K = 30 ε/σ^2 (squares) and K = 100 ε/σ^2 (triangles pointing up) during the equilibration. **(B) Diffusion coefficients.** Compared here are the values of the diffusion coefficients for different spring constants, *i.e.,* K = 5 ε/σ^2 (triangles pointing down), K = 30 ε/σ^2 (squares) and K = 100 ε/σ^2 (triangles pointing up).

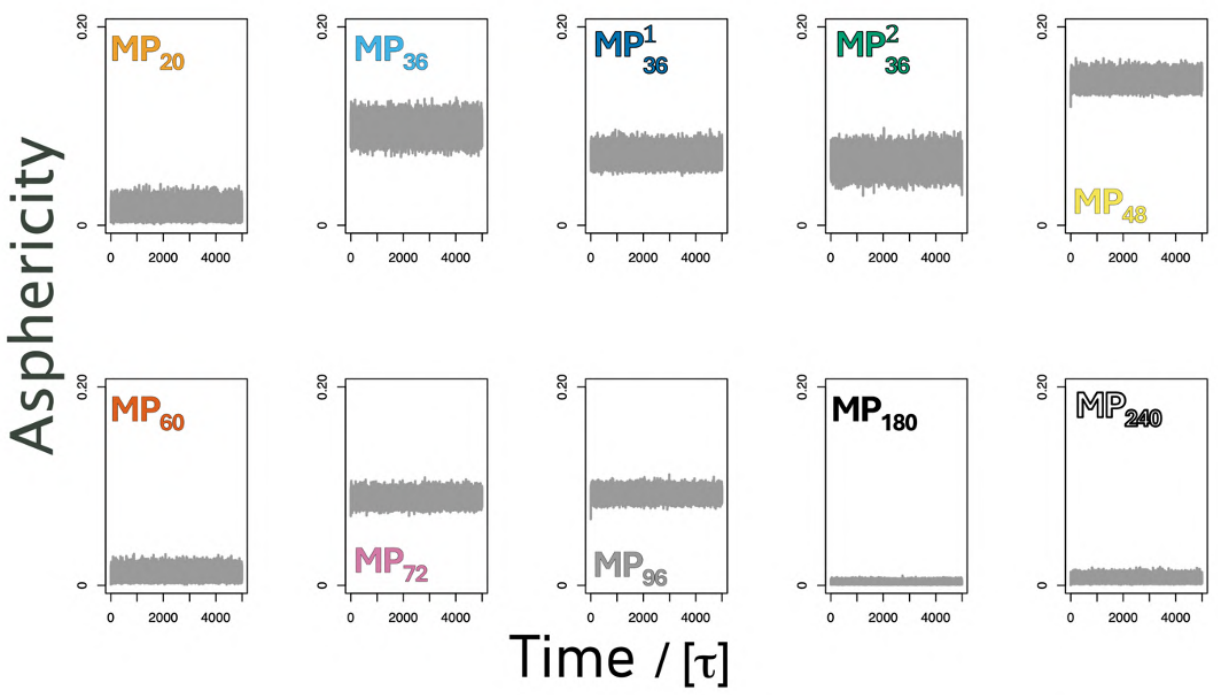

Fig. S2. **Asphericity of the MPs during the equilibration runs.** The asphericity is calculated as $\frac{1}{Rg^2}(\lambda_1 - 0.5 \cdot (\lambda_2 + \lambda_3))$, where λ_1, λ_2, and λ_3 are the eigenvalues (sorted in descending order) of the gyration tensor, and Rg is the radius of gyration. The asphericity is a measure of the shape of a body. Hence, values closer to 0 indicate that the MP has a conformation closer to a sphere, while larger values indicate to which extent the shape of the MP deviates from a sphere. The results align with the sphericity analysis (Fig. 2C) indicating that the MPs with D_{6d} symmetry deviate the most from a spherical shape.

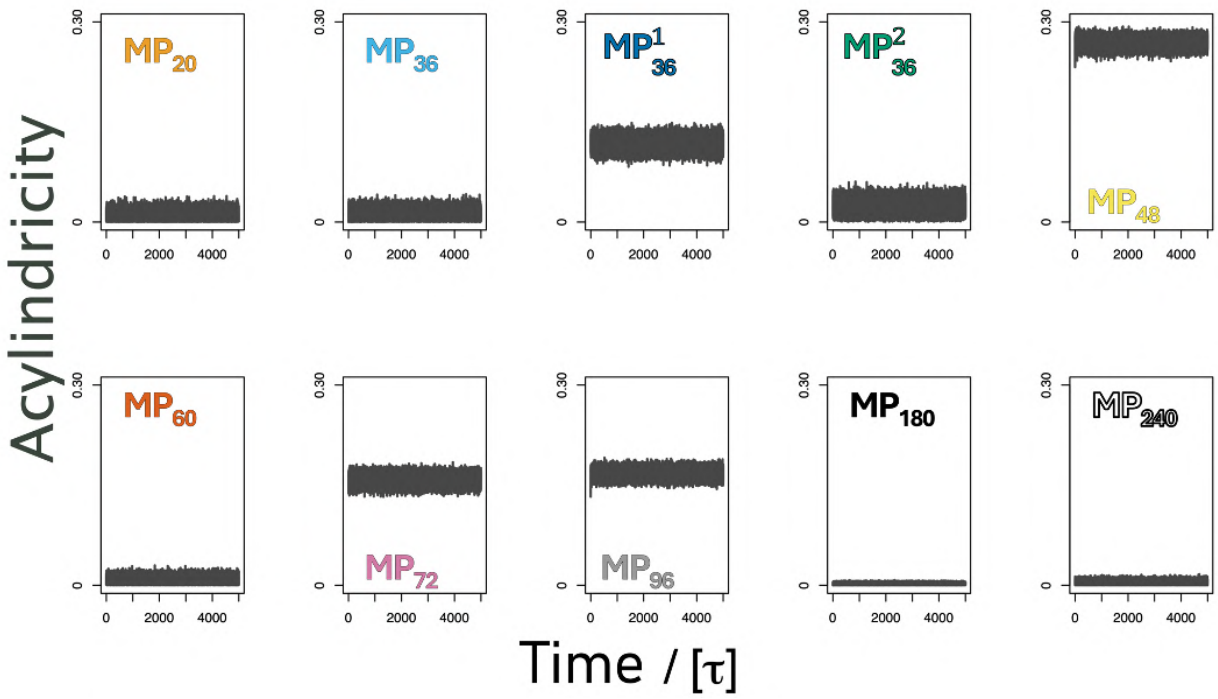

Fig. S3. **Acylindricity of the MPs during the equilibration runs.** The acylindricity is calculated as $\frac{1}{Rg^2}(\lambda_2 - \lambda_3)$, where λ_1, λ_2, and λ_3 are the eigenvalues (sorted in descending order) of the gyration tensor, two of the eigenvalues coincide, and Rg is the radius of gyration. The acylindricity is a measure of the distribution of the beads and resemblance to a cylinder. Hence, it takes values from zero (if all beads are symmetrically arranged) to one (if all beads lie on a line).

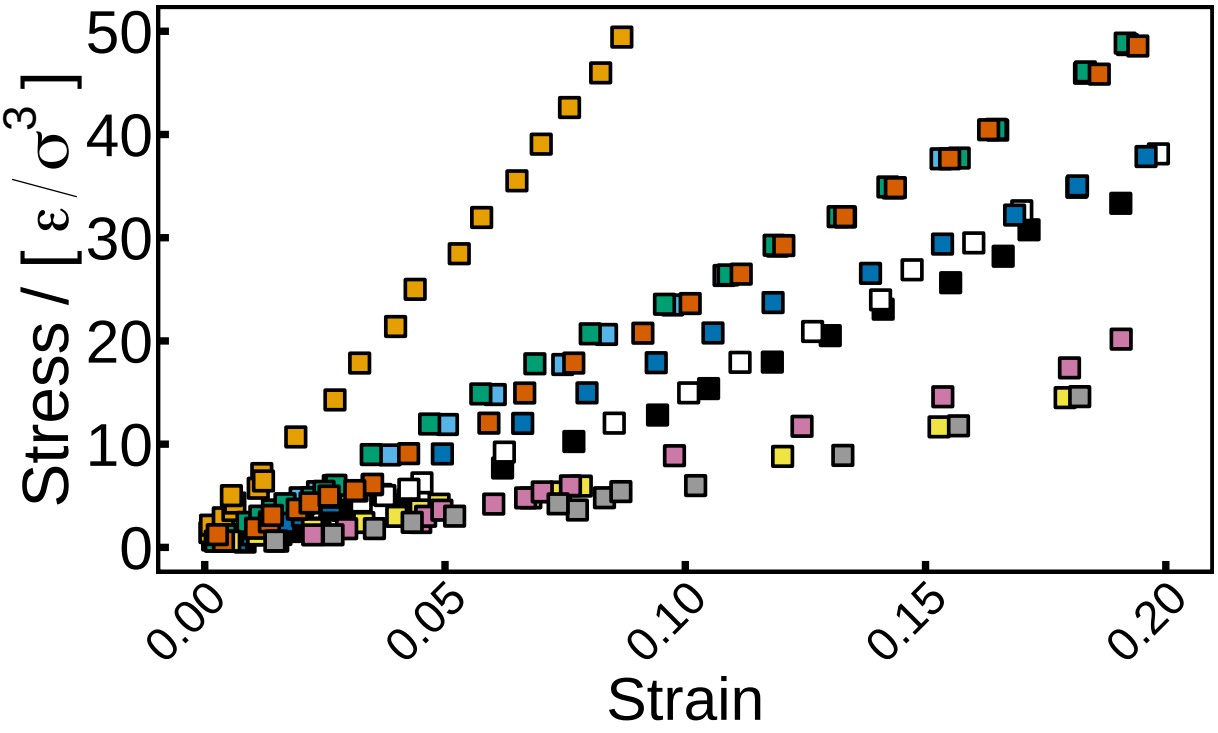

Fig. S4. **Mechanical properties of the metaparticles.** Stress-strain curves zoom-in from Fig. 3A.

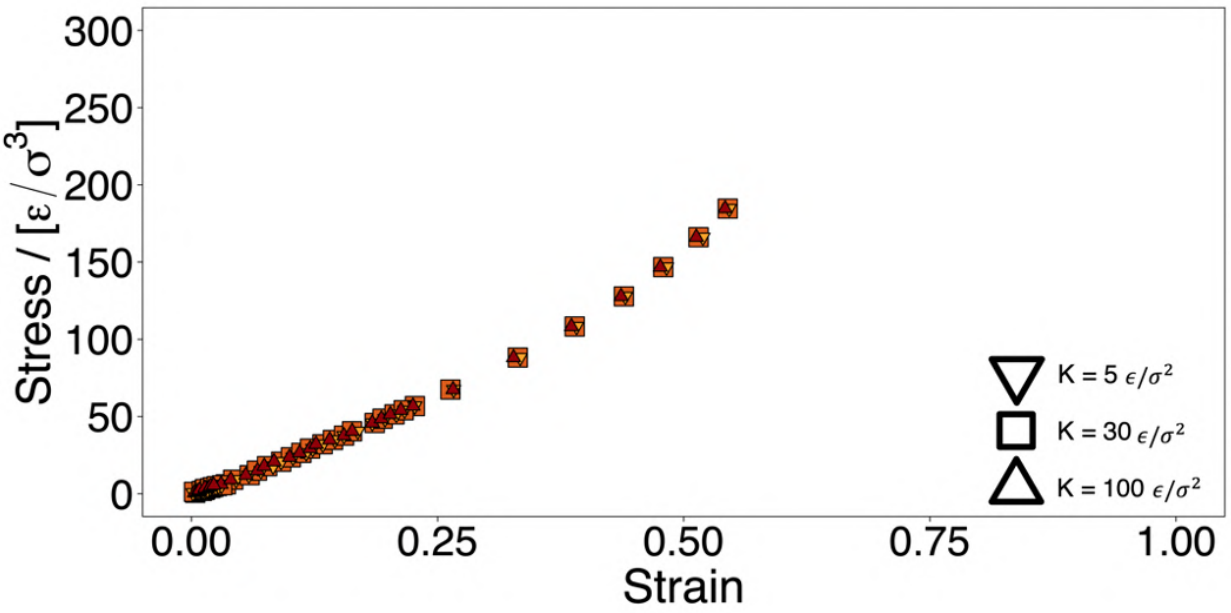

Fig. S5. **Mechanical properties of the metaparticles.** Compared are the stress-strain curves of MP_{60} for different spring constants, *i.e.,* K = 5 ε/σ^2 (triangles pointing down), K = 30 ε/σ^2 (squares) and K = 100 ε/σ^2 (triangles pointing up).

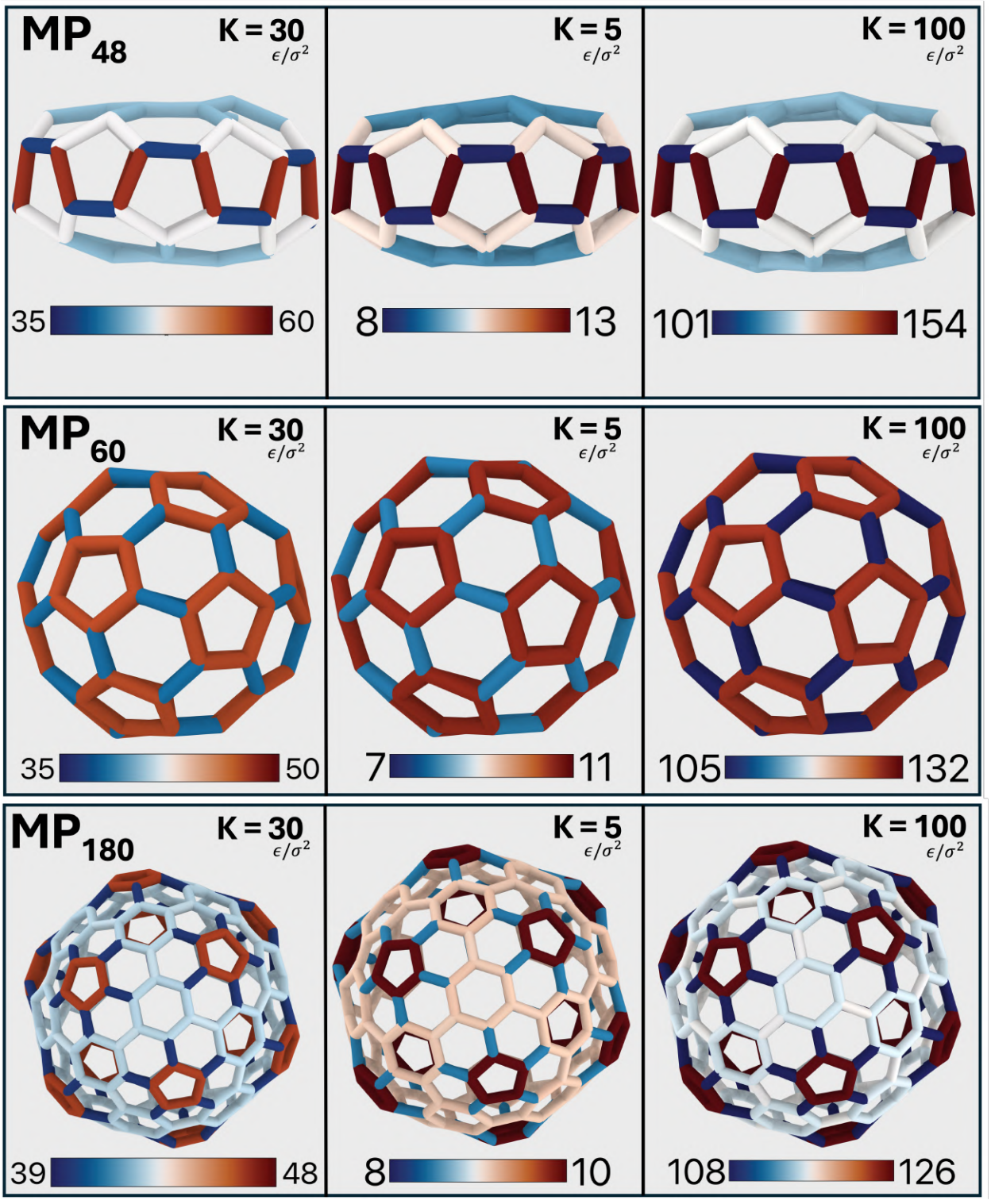

Fig. S6. **Average bond energy distribution** at different values of K during equilibration run for MP_{48}, MP_{60} and MP_{240}.

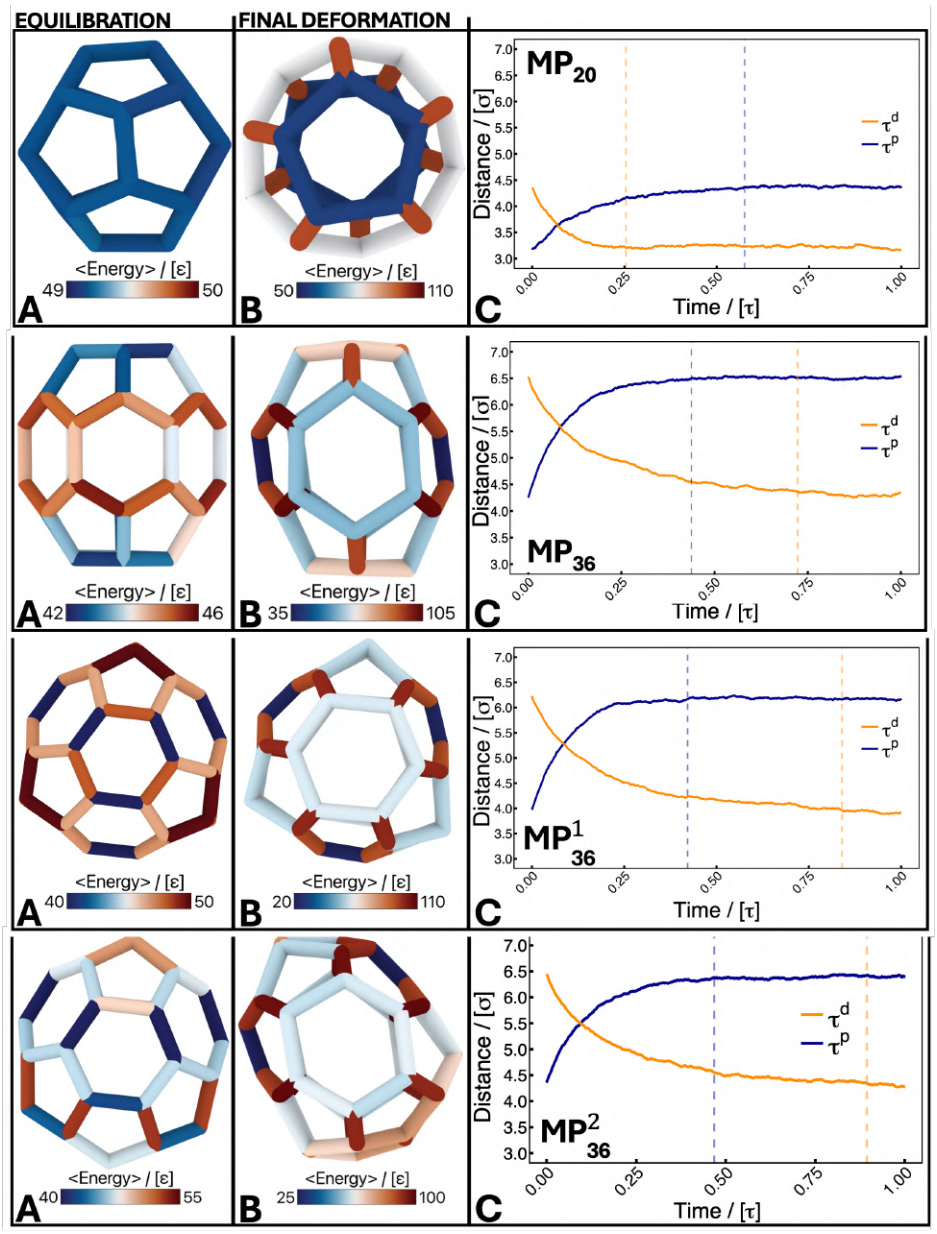

Fig. S7. **Average bond energy distribution** during the equilibration simulation (A) and during the extension simulation (B). The snapshot is a top view of the MP aligned along its deformation axis. Pulling and relaxation timelines (τ^d and τ^r) in blue and orange, respectively (C). The vertical dashed lines represent the times beyond which no additional deformation of the particle is considered. Each individual time has been calculated as the first value that is within the standard deviation of the last 30,000 steps of the simulation. They correspond to the values shown in Fig. 5. Shown are MP_{20}, MP_{36}, MP^1_{36} and MP^2_{36}

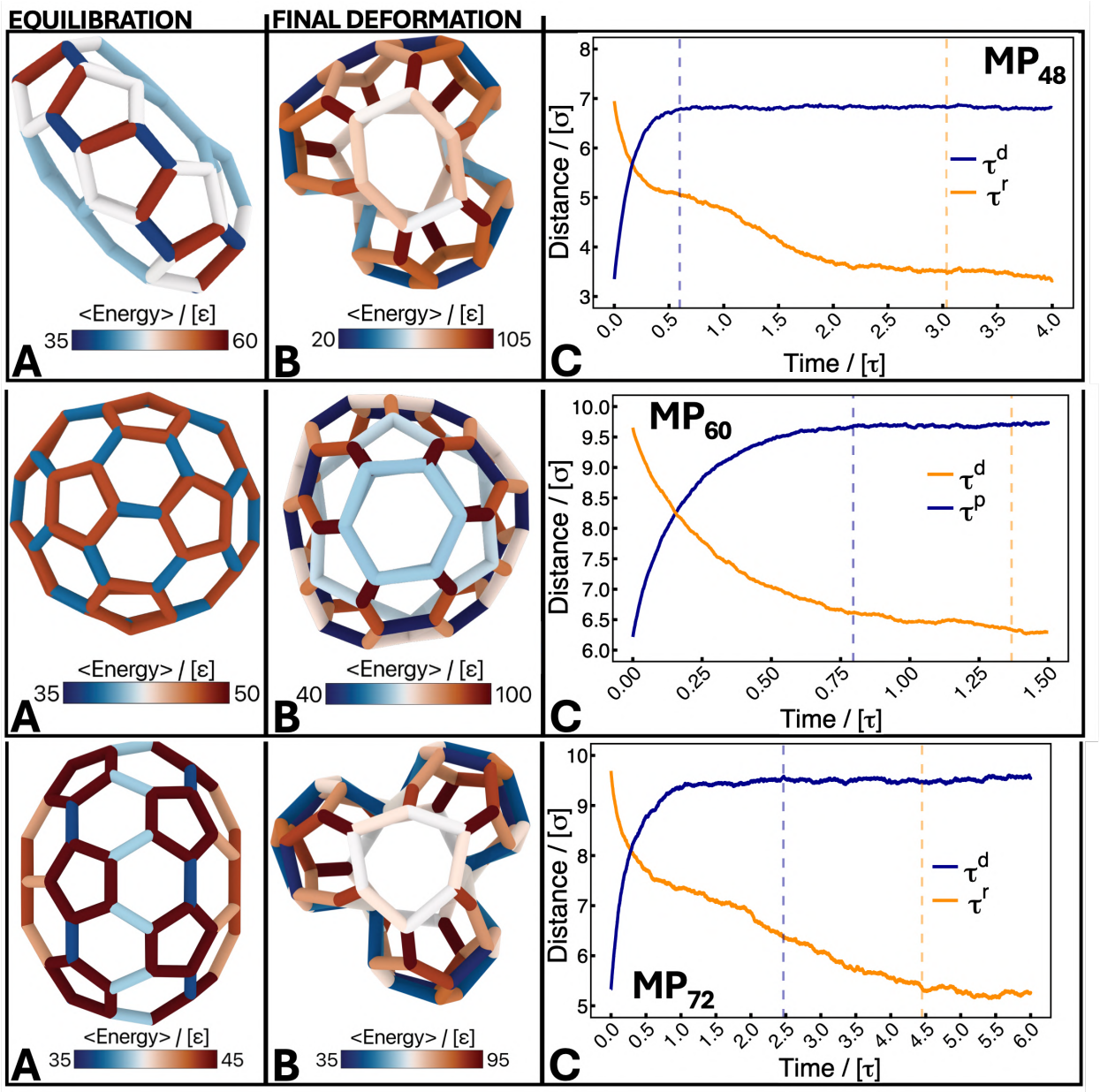

Fig. S8. See Fig. 7. Shown are MP_{48}, MP_{60} and MP_{72}

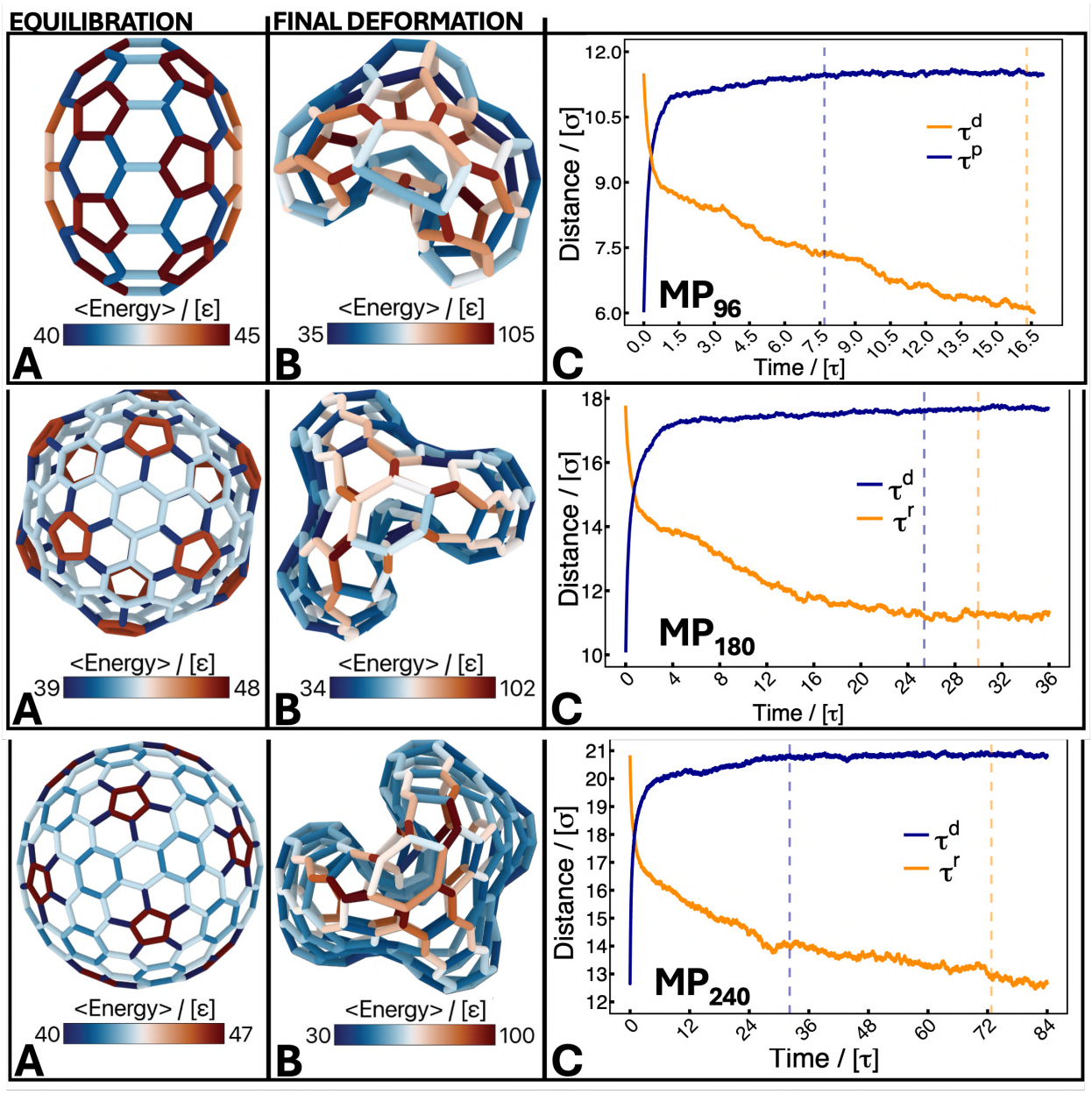

Fig. S9. See Fig. 7. Shown are MP_{96}, MP_{180} and MP_{240}.

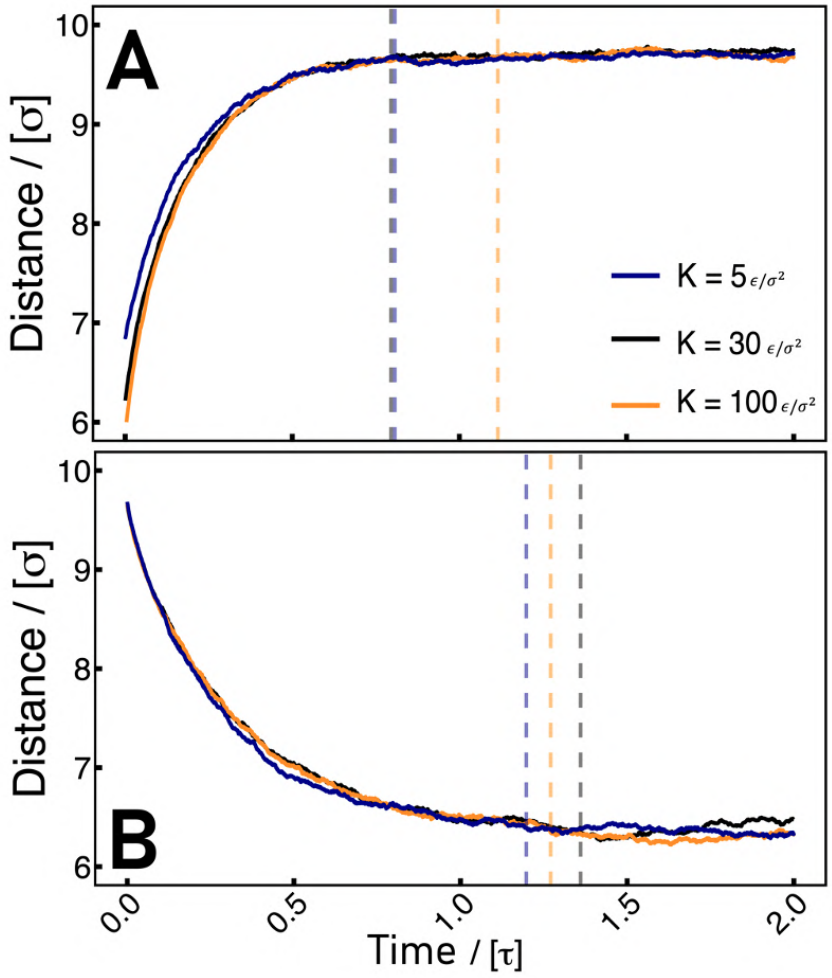

Fig. S10. **Deformation (τ^d) (A) and relaxation times (τ^r) (B) for MP_{60}.** Compared are times required to reach the maximum extension (τ^d) and to relax to the initial conformations (τ^r) for different spring constants, *i.e.,* K = 5 ε/σ^2 (dark blue line), K = 30 ε/σ^2 (black line) and K = 100 ε/σ^2 (dark orange line). For K = 100 ε/σ^2 the time required to reach the maximum extension in highest according to the higher resistance posed by the bonds.